On Schrödinger equation with potential $U = -\alpha r^{-1} + \beta r + kr^2$ and the bi-confluent Heun functions theory

E. Ovsiyuk and O. Veko
Mozyr State Pedagogical University
28 Studencheskaya Str., Mozyr,
247760, Gomel region, Belarus

M. Amirfachrian
Institute of Physics, National Academy of Sciences of Belarus
68 Nezalezhnasci av., Minsk, 220072, Belarus

It is shown that Schrödinger equation with combination of three potentials $U = -\alpha r^{-1} + \beta r + kr^2$, Coulomb, linear and harmonic, the potential often used to describe quarkonium, is reduced to a bi-confluent Heun differential equation. The method to construct its solutions in the form of polynomials is developed, however with additional constraints in four parameters of the model, α, β, k, l. The energy spectrum looks as a modified combination of oscillator and Coulomb parts.

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I. INTRODUCTION

Gauge theories of the strong interactions suggest that the coupling between quarks is weak at short distances but becomes very strong at large distances. This 'explains' the paradox where quarks appear to behave as quasi-free particles within hadrons but cannot be liberated from the hadrons. On the basis of these arguments it was conjectured that heavy quarks would move nonrelativistically within hadrons. Thus bound states of a heavy quark and antiquark should be a hadronic analogue of the positronium system of a bound electron and positron.

This so-called quarkonium system might then be interpreted according to the familiar rules of nonrelativistic quantum mechanics using a potential to describe the interquark force (see [1], [2] and references therein).

At very small distances, the potential is expected to take a form like the Coulomb force, corresponding to the exchange of a single massless gluon. At very large distances, a linear confining potential or something more complex seem to be appropriate. We will use a combination of three well-known potentials

$$U = -\frac{\alpha}{r} + \beta r + kr^2$$

that has some advantages for analytical treatment of the quarkonium problem in terms of Heun functions (this class of special functions being next extension to hypergeometric functions has become of primary importance in many physical problems [3]–[32]).

II. SCHRÖDINGER EQUATION

In Minkowski space, parameterized by spherical coordinate

$$dS^2 = c^2 dt^2 - dr^2 - r^2(d\theta^2 + \sin^2\theta d\phi^2) \; ,$$

the Schrödinger equation for an arbitrary spherical potential has the form

$$i\hbar \frac{\partial}{\partial t}\Psi = \left[-\frac{\hbar^2}{2M} \left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{\hat{l}^{\,2}}{r^2} \right) + U(r) \right] \Psi \; . \tag{1}$$

After separation of the variables, $\Psi = e^{-\frac{iEt}{\hbar}} \, Y_{lm}(\theta,\phi) \, R(r)$, we get

$$E \; R = \left[-\frac{\hbar^2}{2M} \left(\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + U(r) \right] R \; . \tag{2}$$

For a potential specified by (we assume the Coulomb attraction, so $\alpha > 0$)

$$U = -\frac{\alpha}{r} + \beta r + kr^2 \tag{3}$$

eq. (2) reads

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2M}{\hbar^2}\left(E + \frac{\alpha}{r} - \beta r - kr^2\right)\right] R = 0 \, . \tag{4}$$

We may simplify notation by using (instead of (4)) more short form

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + 2\epsilon + \frac{\alpha}{r} - \frac{l(l+1)}{r^2} - \beta r - kr^2\right) R = 0 \tag{5}$$

and further with the substitution $R(r) = r^{-1} f(r)$ we get

$$\left(\frac{d^2}{dr^2} + 2\epsilon + \frac{\alpha}{r} - \frac{l(l+1)}{r^2} - \beta r - kr^2\right) f = 0 \, . \tag{6}$$

Let us see behavior of the curve

$$P^2(r) = 2\epsilon + \frac{\alpha}{r} - \frac{l(l+1)}{r^2} - \beta r - kr^2 \, ,$$
$$P^2(r \sim 0) \sim -\frac{l(l+1)}{r^2} \sim -\infty \, , \qquad P^2(r \sim \infty) \sim -kr^2 - \infty \, .$$

To proceed further, let us examine the classical turning points – the roots of the equation

$$-kr^4 - \beta r^3 + 2\epsilon r^2 + \alpha r - l(l+1) = -k(r - r_1)(r - r_2)(r - r_3)(r - r_4) = 0 \, . \tag{7}$$

From (7) it follows

$$\begin{aligned} -\frac{\beta}{k} &= r_1 + r_2 + r_3 + r_4 \, , \\ -\frac{2\epsilon}{k} &= r_1 r_2 + r_1 r_3 + r_1 r_4 + r_2 r_3 + r_2 r_4 + r_3 r_4 \, , \\ \frac{\alpha}{k} &= r_2 r_3 r_4 + r_1 r_3 r_4 + r_1 r_2 r_4 + r_1 r_2 r_3 \, , \\ \frac{l(l+1)}{k} &= r_1 r_2 r_3 r_4 \, . \end{aligned} \tag{8}$$

There exist the possibility when two roots are negative and two other are positive (see Fig. 1).

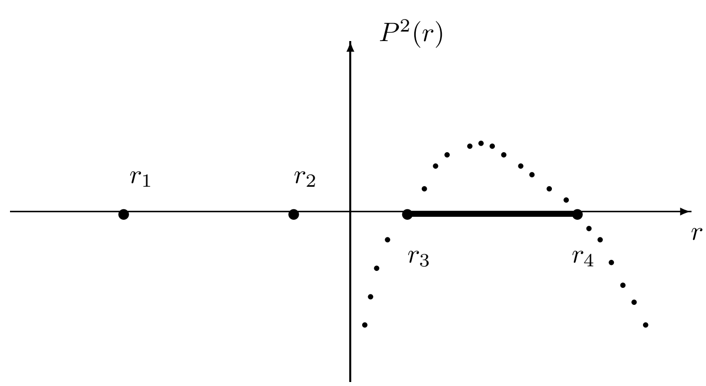

FIG. 1: Finite classical motion at $r \in [r_3, r_4]$

From (7) it follows two systems:

$$-\frac{2\epsilon}{k} = r_1 r_2 + r_1(r_3+r_4) + r_2(r_3+r_4) + r_3 r_4 \,,$$
$$\frac{\alpha}{k} = r_1\, r_3 r_4 + r_2\, r_3 r_4 + r_1 r_2 (r_4 + r_3)\,,$$

and

$$r_1 + r_2 = -\frac{\beta}{k} - r_3 - r_4\,,$$
$$r_1 r_2 = \frac{l(l+1)}{k\, r_3 r_4}\,.$$

Making the change of variables $y = iKr$ ($K = k^{1/4}$):

$$\frac{d^2R}{dy^2} + \frac{2}{y}\frac{dR}{dy} - \left(\frac{2\epsilon}{K^2} + \frac{i\alpha}{Ky} + \frac{l(l+1)}{y^2} + \frac{i\beta y}{K^3} + y^2\right) R = 0 \tag{9}$$

and using the substitution

$$R = y^A\, e^{By}\, e^{Cy^2} F(y)\,, \tag{10}$$

we get

$$\frac{d^2F}{dy^2} + \left[\frac{2(A+1)}{y} + 4Cy + 2B\right]\frac{dF}{dy} + \left[(4C^2-1)\,y^2 + \left(4BC - \frac{i\,\beta}{K^3}\right) y + \right.$$
$$\left. + 4AC + B^2 - \frac{2\epsilon}{K^2} + 6C + \frac{A^2 + A - l(l+1)}{y^2} + \frac{2ABK + 2BK - i\alpha}{y\,K}\right] F = 0\,. \tag{11}$$

With the choice of special values

$$A = +l\,,\ -(l+1)\,, \qquad C = \pm\frac{1}{2}\,, \qquad B = \pm\frac{i\beta}{2\,K^3}\,, \tag{12}$$

take those related to possible bound states

$$A = +l, \qquad y^A \sim r^l\,;$$
$$C = +\frac{1}{2}\,, \qquad e^{Cy^2} = e^{-K^2 r^2/2}\,;$$
$$B = +\frac{i\beta}{2\,K^3}\,, \qquad e^{By} = e^{-\beta r/2K^2}\,; \tag{13}$$

eq. (11) becomes simpler

$$\frac{d^2F}{dy^2} + \left[\frac{2(A+1)}{y} + 4Cy + 2B\right]\frac{dF}{dy} +$$
$$+ \left[4AC + B^2 - \frac{2\epsilon}{K^2} + 6C + \frac{2ABK + 2BK - i\alpha}{y\,K}\right] F = 0\,. \tag{14}$$

It is convenient to turn to the variable

$$z = \frac{y}{i} = Kr\,;$$

then eq. (14) reads (remember that $A = +l$ $\;C = +1/2$)

$$\frac{d^2F}{dz^2} + \left(-2z + 2iB + \frac{1 + (2l+1)}{z}\right)\frac{dF}{dz} +$$
$$+ \left(-2 - (2l+1) + (\frac{2\epsilon}{K^2} - B^2) + \frac{-(-2iB)(l+1) + \alpha/K}{z}\right) F = 0\,, \tag{15}$$

which can be recognized as a biconfluent Heun equation for functions $H(a,b,c,d,z)$

$$\frac{d^2H}{dz^2}+\left(-2z-b+\frac{1+a}{z}\right)\frac{dH}{dz}+\left(-2-a+c+\frac{-b(a+1)/2-d/2}{z}\right)H=0 \tag{16}$$

with parameters

$$a=2l+1\,,\qquad b=-2iB=\frac{\beta}{K^3}\,,\qquad c=\frac{2\epsilon}{K^2}+\frac{\beta^2}{4K^6}\,,\qquad d=-\frac{2\,\alpha}{K}\,. \tag{17}$$

Let us present solutions of eq. (16) as a series

$$H(z)=1+c_1z+c_2z^2+c_3z^3+...=\sum_{n=0}^{\infty}c_nz^n\;,$$

$$H'(z)=c_1+2c_2z^1+3c_3z^2+...=\sum_{n=1}^{\infty}nc_nz^{n-1}\;,$$

$$H''(z)=2\times 1\;c_2z^0+3\times 2\;c_3z^1+...=\sum_{n=2}^{\infty}n(n-1)c_nz^{n-2}\;.$$

Eq. (16) gives (let $D=-b(a+1)/2-d/2$)

$$\frac{d^2H}{dz^2}+\left(-2z-b+\frac{1+a}{z}\right)\frac{dH}{dz}+\left(-2-a+c+\frac{D}{z}\right)H=0\;;$$

that is

$$\begin{gathered}\sum_{n=2}^{\infty}n(n-1)c_nz^{n-2}+\\+(-2z-b+\frac{1+a}{z})\sum_{n=1}^{\infty}nc_nz^{n-1}+\\+(-2-a+c+\frac{D}{z})\sum_{n=0}^{\infty}c_nz^n=0\;.\end{gathered} \tag{18}$$

From (18) it follows

$$\sum_{n=2}^{\infty}n(n-1)c_nz^{n-2}-\sum_{n=1}^{\infty}2nc_nz^n-\sum_{n=1}^{\infty}bnc_nz^{n-1}+$$
$$+\sum_{n=1}^{\infty}(1+a)nc_nz^{n-2}+\sum_{n=0}^{\infty}(-2-a+c)c_nz^n+\sum_{n=0}^{\infty}Dc_nz^{n-1}$$

or

$$\sum_{N=0}^{\infty}(N+2)(N+1)c_{N+2}z^N-\sum_{N=1}^{\infty}2Nc_Nz^N-\sum_{N=0}^{\infty}b(N+1)c_{N+1}z^N+$$
$$+\sum_{N=-1}^{\infty}(1+a)(N+2)c_{N+2}z^N+\sum_{N=0}^{\infty}(-2-a+c)c_Nz^N+\sum_{N=-1}^{\infty}Dc_{N+1}z^N\;.$$

Collecting similar terms

$$
\begin{aligned}
2c_2 + \sum_{N=1}^{\infty} (N+2)(N+1) c_{N+2} z^N - \\
- \sum_{N=1}^{\infty} 2N c_N z^N - b c_1 - \sum_{N=1}^{\infty} b(N+1) c_{N+1} z^N + \\
+(1+a) c_1 z^{-1} + (1+a) 2 c_2 + \sum_{N=1}^{\infty} (1+a)(N+2) c_{N+2} z^N + \\
+(-2-a+c) c_0 + \sum_{N=1}^{\infty} (-2-a+c) c_N z^N + \\
+D c_0 z^{-1} + D c_1 + \sum_{N=1}^{\infty} D c_{N+1} z^N = 0
\end{aligned}
$$

we get

$$
\begin{aligned}
[\ (1+a) c_1 + D c_0]\ z^{-1} + \\
+ [\ 2c_2 - b c_1 + (1+a) 2 c_2 + (-2-a+c) c_0 + D c_1\ ] + \\
+ \sum_{N=1}^{\infty} [\ (N+2)(N+1) c_{N+2} - 2N c_N - b(N+1) c_{N+1} + \\
+(1+a)(N+2) c_{N+2} + (-2-a+c) c_N + D c_{N+1}\ ]\ z^N = 0\,.
\end{aligned}
$$

Thus we arrive at the recurrent relations for series coefficients

$$
\begin{gathered}
c_1 = -\frac{D}{(1+a)}\, c_0\,, \qquad c_2 = \frac{(2+a-c) c_0 + (b-D) c_1}{(a+2)2}\,, \\
c_{N+2} = \frac{(2N+2+a-c)\ c_N + [-D + b(N+1)]\ c_{N+1}}{(N+2)(a+N+2)}\,, \qquad N = 1, 2, ...
\end{gathered} \tag{19}
$$

From this, after simple change in notation, we obtain

$$
\begin{gathered}
c_1 = -\frac{D}{(1+a)}\, c_0\,, \qquad c_2 = \frac{(2+a-c) c_0 + (b-D) c_1}{(a+2)2}\,, \\
c_{n+1} = \frac{(2n+a-c)\ c_{n-1} + (-D + bn)\ c_n}{(n+1)(a+n+1)}\,, \qquad n = 2, 3, 4, ...
\end{gathered} \tag{20}
$$

Remember that

$$
a = 2l + 1\,, \qquad b = \frac{\beta}{K^3}\,, \qquad d = -\frac{2\,\alpha}{K} \qquad c = \frac{2\epsilon}{K^2} + \frac{b^2}{4}\,,
$$

we obtain

$$
\begin{gathered}
-D = b(l+1) - \frac{\alpha}{K}\,, \qquad b - D = b(l+2) - \frac{\alpha}{K}\,, \\
2b - D = b(l+3) - \frac{\alpha}{K}\,, \ \ ... \ \ bn - D = b(l+n+1) - \frac{\alpha}{K}\,;
\end{gathered} \tag{21}
$$

note that the energy parameter does not enter relations in (2.17), instead it is presented only in the parameter c

$$
c = \frac{2\epsilon}{K^2} + \frac{b^2}{4}\,. \tag{22}
$$

Recursive relation can be rewritten in the form

$$c_1 = -\frac{D}{2(2l+2)}\, c_0 \, ,$$
$$c_2 = \frac{[\, (2(l+1) + (1-c)\,]\, c_0 + (b-D)c_1}{2\,[(2(l+1)+1]} \, ,$$
$$c_3 = \frac{[\, 2(l+2) + (1-c)\,]\, c_1 + (2b-D)\, c_2}{3\,[2(l+1)+2]} \, ,$$
$$c_4 = \frac{[\, 2(3+l) + (1-c)\,]\, c_2 + (3b-D)\, c_3}{4\,[\, 2(l+1)+3]} \, ,$$
$$c_5 = \frac{[\, 2(4+l) + (1-c)\,]\, c_3 + (4b-D)\, c_4}{5\,[\, 2(l+1)+4]} \, ,$$

. . . .

$$c_{n+1} = \frac{[\, 2(n+l) + (1-c)\,]\, c_{n-1} + (nb-D)\, c_n}{(n+1)\,[\, 2(l+1)+n]} \, ... \tag{23}$$

Ont can try to obtain polynomial solutions. The first simplest possibility can be realized by adding two constraints:

$$c_1 = 0, \qquad c_2 = 0 \tag{24}$$

which gives

$$D = 0 \qquad \Longrightarrow \qquad \frac{\beta(l+1)}{K^2} = \alpha \, ,$$
$$c = (2(l+1)+1 \qquad \Longrightarrow \qquad \frac{2\epsilon}{K^2} + \frac{b^2}{4} = 2(l+1)+1 \, . \tag{25}$$

Result (25) may be rewritten as follows
<u>the case $n = 0$</u>

$$\epsilon = K^2(l+1+\frac{1}{2}) - \frac{1}{8}(\frac{\alpha}{l+1})^2 \, , \qquad \text{where} \qquad \frac{\alpha}{l+1} = \frac{\beta}{K^2} \, . \tag{26}$$

Let us consider the case $n = 1$ which is realized by adding two constraints

$$c_2 = 0 \, , \qquad [\, (2(l+1) + (1-c)\,]\, c_0 + (b-D)c_1 = 0 \, ,$$
$$c_3 = 0 \, , \qquad 2(l+2) + (1-c) = 0 \, , \tag{27}$$

which leads to

$$c = 2(l+2)+1 \, ,$$
$$2 + (b-D)\frac{D}{2(2l+2)} = 0 \, . \tag{28}$$

In explicit form they are

$$\frac{2\epsilon}{K^2} + \frac{b^2}{4} = 2(l+2)+1 \, , \tag{29}$$

and

$$4(2l+2) - [-\frac{\alpha}{K} + b(l+2)][-\frac{\alpha}{K} + b(l+1)] = 0 \, . \tag{30}$$

Eq. (30) is a 2-order equation with respect to b

$$b^2(l+1)(l+2) - b\frac{\alpha}{K}(2l+3) - 4(2l+2) + \frac{\alpha^2}{K^2} = 0$$

with its solution

$$b = +\frac{\alpha}{K}\frac{(l+3/2)}{(l+1)(l+2)} \pm \left[(\frac{\alpha}{K})^2 \left(\frac{(l+3/2)}{(l+1)(l+2)} \right)^2 + \frac{4(2l+2) - \alpha^2/K^2}{(l+1)(l+2)} \right]^{1/2}$$

or

$$b = +\frac{\alpha}{K}\frac{(l+3/2)}{(l+1)(l+2)} \pm \sqrt{ (\frac{\alpha}{K})^2 \frac{1/4}{(l+1)^2(l+2)^2} + \frac{8}{(l+2)} } \; . \tag{31}$$

Let us consider several first coefficients of the bi-confluent Heun series:

$$\begin{aligned}
c_1 &= -\frac{D}{2(2l+2)}\, c_0 \; ; \\
c_2 &= \frac{(2(l+1)+(1-c)}{2\,[\,(2(l+1)+1\,]}\, c_0 + \frac{(b-D)}{2\,[\,(2(l+1)+1\,]}\, c_1 = \\
&= \frac{(2(l+1)+(1-c)}{2\,[\,(2(l+1)+1\,]}\, c_0 + \frac{(b-D)}{2\,[\,(2(l+1)+1\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) \; ; \\
c_3 &= \frac{2(l+2)+(1-c)}{3\,[\,2(l+1)+2\,]}\, c_1 + \frac{(2b-D)}{3\,[\,2(l+1)+2\,]}\, c_2 = \\
&= \frac{2(l+2)+(1-c)}{3\,[\,2(l+1)+2\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) + \\
&+ \frac{(2b-D)}{3\,[\,2(l+1)+2\,]} \left[\frac{(2(l+1)+(1-c)}{2\,[\,(2(l+1)+1\,]}\, c_0 + \frac{(b-D)}{2\,[\,(2(l+1)+1\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) \right] \; ; \\
c_4 &= \frac{2(3+l)+(1-c)}{4\,[\,2(l+1)+3]}\, c_2 + \frac{(3b-D)}{4\,[\,2(l+1)+3]}\, c_3 = \\
&= \frac{2(3+l)+(1-c)}{4\,[\,2(l+1)+3]} \left[\frac{(2(l+1)+(1-c)}{2\,[\,(2(l+1)+1\,]}\, c_0 + \frac{(b-D)}{2\,[\,(2(l+1)+1\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) \right] + \\
&+ \frac{(3b-D)}{4\,[\,2(l+1)+3]} \left\{ \frac{2(l+2)+(1-c)}{3\,[\,2(l+1)+2\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) + \right. \\
&\left. + \frac{(2b-D)}{3\,[\,2(l+1)+2\,]} \left[\frac{(2(l+1)+(1-c)}{2\,[\,(2(l+1)+1\,]}\, c_0 + \frac{(b-D)}{2\,[\,(2(l+1)+1\,]} \left(-\frac{D}{2(2l+2)}\, c_0 \right) \right] \right\} \; ;
\end{aligned}$$

. . . .

The coefficient c_n represents a n-polynomial with respect to parameter b.

In principle, it is easily to extend the above polynomial-based approach to general case. Indeed, let it be

$$c_{n+1} = 0 \, , \qquad c_{n+2} = 0 \, , \tag{32}$$

which gives

$$\begin{aligned}
c_{n+1} = 0, \qquad [\,2(n+l) + (1-c)\,]\, c_{n-1} + (nb - D)\, c_n = 0 \, , \\
c_{n+2} = 0, \qquad [\,2(n+1+l) + (1-c)\,]\, c_n = 0 \, .
\end{aligned} \tag{33}$$

From whence it follows

$$\begin{aligned}
(1-c) = -2(n+1+l) \, , \\
-2c_{n-1} + (nb - D)\, c_n = 0 \, .
\end{aligned} \tag{34}$$

The problem is reduced to rather complicated polynomials. This method provides us with the formula for energy levels; however we obtain some additional constraints for four parameters, α, β, k, l (in the form of n-polynomial). This means that we are able to construct solutions in the polynomial form, but only at some special values of α, β, k, l.

General structure of the 3-term recurrent relations can be presented in a more short notation

$$\begin{aligned}
c_1 &= A_0 c_0 \ , \\
c_2 &= E_0 c_0 + A_1 c_1 \ , \\
c_3 &= E_1 c_1 + A_2 c_2 \ , \\
c_4 &= E_2 c_2 + A_3 c_3 \ , \\
c_5 &= E_3 c_3 + A_4 c_4 \ , \\
& \ldots\ldots\ldots\ldots\ldots\ldots \\
c_{n+1} &= E_{n-1} c_{n-1} + A_n c_n \ , \\
& \ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned} \tag{35}$$

where

$$E_{n-1} = \frac{2(n+l) + (1-c)}{(n+1)\ [\ 2(l+1) + n]}, \qquad A_n = \frac{(nb - D)}{(n+1)\ [\ 2(l+1) + n]} \ . \tag{36}$$

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